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The difference between the defect and local relaxation problems on one band and the perfect lattice problem on

$$P_{\mu' s \lambda' t} = 2 \int \sum^{\sigma_{\mathrm{occ}}} C^{*}_{\mu' \gamma s}(\mathbf{K}_p) C_{\lambda' \gamma t}(\mathbf{K}_p) \exp[i\mathbf{K}_p \cdot (\mathbf{R}_s - \mathbf{R}_t)] d\mathbf{K}_p ,$$

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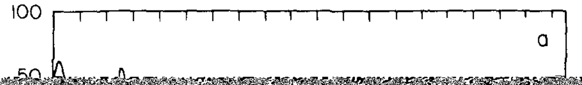
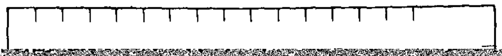
FIG. 2. Planar zigzag chain forming the crystal structure of solid HF. Intramolecular

charge is shown in Figs. 6a and 6b, respectively. Four to five neighbors are sufficient to obtain the cohesive energy to within less than 0.1 kcal/mole from the con-





overestimated by 2.5 eV, and the valence band is wider by 1.8 eV. The atomic charge of the central atom in

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plane angles, chain angle, and $R_{HF}$ keeping $R_{FF}$ constant at the experimental value), against displacement of a specific proton. Figure 17 shows the variation in

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